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Analytic expression for three-body recombination rates into deep dimers

Abstract We investigate three-body recombination rates into deep dimers in cold atomic gases with large scattering length within hyper-spherical adiabatic zero-range approach. We derive closed analytic expressions for the rates for one- and two-species gases. Although the deep dimers are beyond the zero-range theory the latter can still describe the recombination into deep dimers by use of one additional short-range absorption parameter. The recombination rate, as function of the scattering length, retains the known universal behavior — the fourth power trend with characteristic log-periodic peaks — however increasing the short-range absorption broadens the peaks until they are eventually completely smeared out. Increasing the heavy-to-light mass ratio in a two-species system decreases the distance between the peaks and increases the overall scale of the recombination rate.

1 Introduction

Three-body recombination is the principal source of loss of atoms in a trapped cold atomic gas. The loss rates are directly measurable as functions of the tunable interaction parameters. A number of recent experiments have provided results for various combinations of alkali atoms [1,6,10].

The recombination reaction can conclude with either a shallow — weakly bound — dimer, or with a deep — strongly bound — dimer. The recombination rates into shallow dimers in cold atomic gases with large scattering length exhibit the well-known universal behavior — the rates, as function of the scattering length, show the fourth power trend with the characteristic log-periodic structures [8,3,11]. This behavior is universal — it can be described by a zero-range theory with only one parameter, the scattering length. The universal behavior is the consequence of the fact that for cold atoms with large scattering lengths both the three-body dynamics and the shallow dimers depend only on the long distance properties of the atomic interaction which is largely determined by the scattering length alone.

The deep dimers, on the contrary, cannot be described by a zero-range — a long distance — theory as their properties depend on the short distance physics. For a long distance theory the recombination into deep dimers, which takes place at short distances, looks simply like a sink of probability at short distances. Therefore in zero-range theories the recombination into deep dimers can be described phenomenologically by introducing one extra parameter which creates such a sink of probability [2,9,7,12].

We shall follow this philosophy — to introduce an extra phenomenological parameter to account for the loss of probability at short distances — and calculate the recombination rates as function of scattering length within a hyper-spherical adiabatic zero-range theory.

What distinguishes us from previous investigations is that we derive a closed analytic expression which works for both one- and two-species cold gases.

2 Zero-range model

2.1 Hyper-spherical adiabatic approximation

Within the zero-range hyper-spherical adiabatic approximation [4, 5] the wave-function of the three-body system is written as

$$\Psi(\rho, \Omega_\rho) = \rho^{-\frac{5}{2}} f(\rho) \Phi(\rho, \Omega_\rho), \quad (1)$$

where the hyper-radius ρ and the hyper-angles Ω_ρ are defined in appendix A. The hyper-radial function $\Phi(\rho, \Omega_\rho)$ is normalized to one in hyper-angles and for large ρ loses its dependence on ρ and turns into a hyper-spherical harmonic. Its exact form is of no importance in the present context.

The hyper-radial function $f(\rho)$ satisfies the hyper-radial equation

$$\left(-\frac{d^2}{d\rho^2} + \frac{\nu^2(\rho) - \frac{1}{4}}{\rho^2} - \frac{2mE}{\hbar^2} \right) f(\rho) = 0, \quad (2)$$

where m is the mass-scale from the definition (31) of the hyper-radial coordinates, E is the energy of the three-body system, and $\nu(\rho)$ is the angular eigenvalue given by the lowest root of the angular eigenvalue equation. The latter depends on the scattering lengths and masses of the particles.

For a system of three identical particles — which corresponds to a *one-species cold gas* — the eigenvalue-equation is given as

$$-\nu \cos\left(\frac{\nu\pi}{2}\right) + \frac{8}{\sqrt{3}} \sin\left(\frac{\nu\pi}{6}\right) = \frac{1}{\sqrt{\mu_1}} \left(\frac{\rho}{-a_1} \right) \sin\left(\frac{\nu\pi}{2}\right), \quad (3)$$

where $a_1 < 0$ is the scattering length¹ and μ_1 is dimensionless reduced mass from the definition (31) of the hyper-spherical coordinates².

For a *two-species cold gas* we shall consider the common situation with one light particle with mass m_3 and two identical heavy particles with masses $m_1 = m_2$. We shall assume that only the scattering lengths between the light and the heavy particles, $a_1 = a_2$, are large and that the scattering length a_3 between the heavy particles is, in comparison, negligibly small. In this case the angular eigenvalue equation is given as

$$-\nu \cos\left(\frac{\nu\pi}{2}\right) - \frac{2}{\sin(2\phi_{12})} \sin\left[\nu\left(\phi_{12} - \frac{\pi}{2}\right)\right] = \frac{1}{\sqrt{\mu_1}} \left(\frac{\rho}{-a_1} \right) \sin\left(\frac{\nu\pi}{2}\right), \quad (4)$$

where

$$\phi_{12} = \arctan\left(\sqrt{\frac{m_3(m_1 + m_2 + m_3)}{m_1 m_2}}\right). \quad (5)$$

The shape of the effective potential in the hyper-radial equation (2) for one- and two-species systems is illustrated on Fig. 1: it features an attractive pocket at short distances followed by a repulsive barrier at long distances — an archetypal shape, conducive to narrow resonances behind a barrier.

The dividing point, ρ_0 , between the two regions is located where the effective potential is equal zero, that is, given by the solution to the equation $\nu(\rho_0) = \frac{1}{2}$. For the one-species system

$$\rho_0 \approx 0.84|a_1|. \quad (6)$$

For two-species systems we find the following numerical approximation to ρ_0 as function of the heavy-to-light mass ratio m_1/m_3 in the practically relevant region of mass ratios,

$$\frac{\rho_0}{|a_1|} \approx 0.29 \left(\frac{m_1}{m_3} \right)^{0.69}. \quad (7)$$

The quality of the approximation is illustrated on Fig. 2.

¹ We use the atomic-physics sign convention where the absence of the shallow dimer corresponds to negative scattering length.

² For three identical particles we choose $m = m_1 = m_2 = m_3$ and, consequently, $\mu_1 = \frac{1}{2}$.

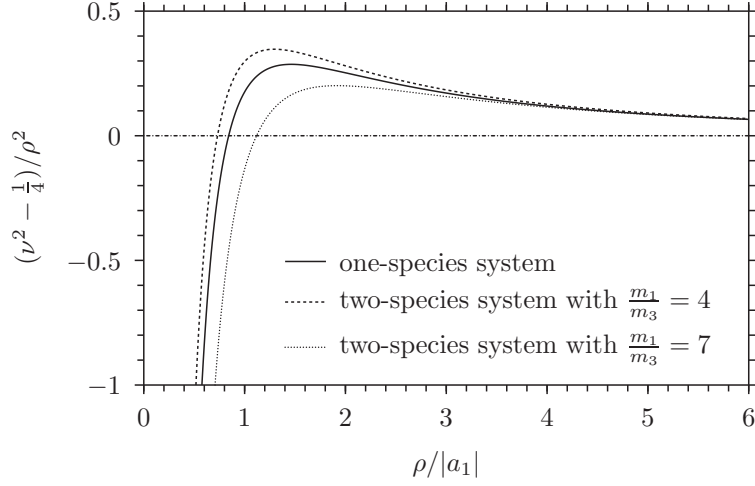


Fig. 1 The effective potential, $(\nu^2 - \frac{1}{4})/\rho^2$, in the hyper-radial equation (2) for one- and two-species systems.

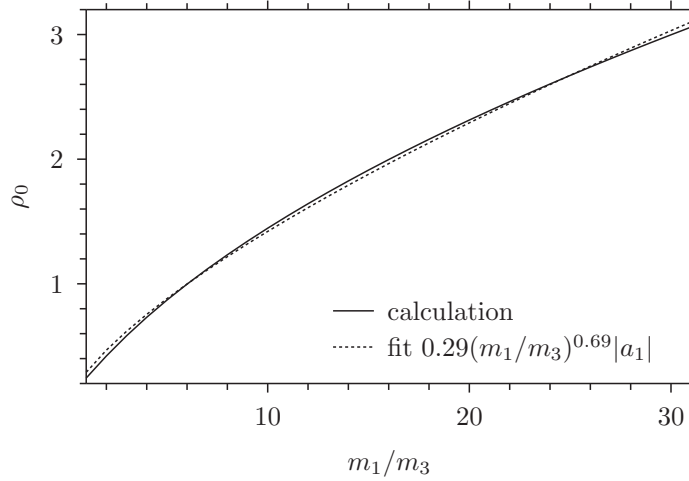


Fig. 2 The solution ρ_0 to equation $(\nu(\rho_0)^2 - \frac{1}{4}) = 0$ for two-species system as function of the heavy-to-light mass ratio m_1/m_3 together with a phenomenological fit.

2.2 Asymptotic regions

In the long-distance region, $\rho \gg |a_1|$, the solution to eigenvalue-equations for both one- and two-species systems is $\nu = 2$. This leads to an asymptotic equation with a (half-integer) centrifugal barrier,

$$\left(-\frac{d^2}{d\rho^2} + \frac{4 - \frac{1}{4}}{\rho^2} - \frac{2mE}{\hbar^2} \right) f(\rho) = 0, \quad (8)$$

with the solution

$$\rho^{-\frac{1}{2}} f(\rho) = J_2(\kappa\rho) - \tan(\delta) Y_2(\kappa\rho), \quad (9)$$

where $J_2(\kappa\rho)$, $Y_2(\kappa\rho)$ are the regular and irregular Bessel functions, $\hbar\kappa = \sqrt{2mE}$, and δ is the phase-shift determined by the physics at short distances.

In the short-distance region, $\rho \ll |a_1|$, the eigenvalue-equation (3) for the one-species system reduces to

$$-\nu \cos\left(\frac{\nu\pi}{2}\right) + \frac{8}{\sqrt{3}} \sin\left(\frac{\nu\pi}{6}\right) = 0, \quad (10)$$

which has an imaginary root $\nu = is$ where $s \approx 1.006$.

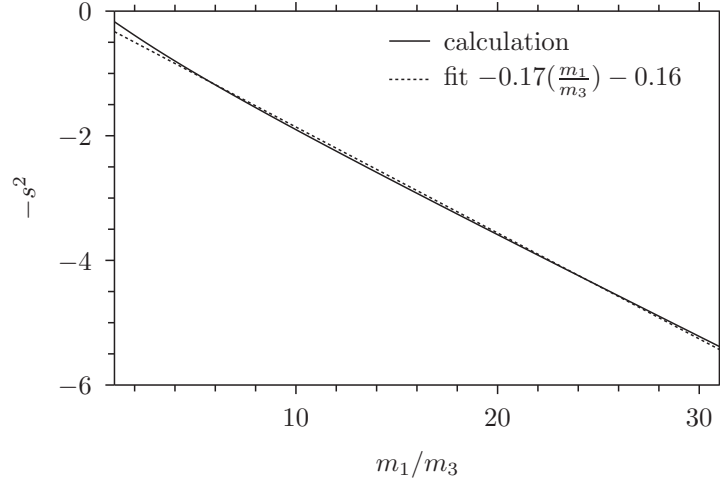


Fig. 3 The square, $\nu(0)^2 \doteq -s^2$, of the solution to the short-distance eigenvalue equation (11) for two-species system as function of the heavy-to-light mass ratio m_1/m_3 , together with a phenomenological fit.

The eigenvalue equation (4) for two-species system in the short-distance region $\rho \ll |a_1|$ reduces to

$$-\nu \cos\left(\frac{\nu\pi}{2}\right) - \frac{2}{\sin(2\phi_{12})} \sin\left[\nu\left(\phi_{12} - \frac{\pi}{2}\right)\right] = 0, \quad (11)$$

which also has an imaginary root $\nu = is$. However, the parameter s now depends on the heavy-to-light mass ratio m_1/m_3 as illustrated on Fig. 3: increasing mass ratio increases s , and thus the attraction at short distances.

Thus for both one- and two-species systems the hyper-radial equation at short distances acquires a super-attractive effective potential,

$$\left(-\frac{d^2}{d\rho^2} + \frac{-s^2 - \frac{1}{4}}{\rho^2}\right) f(\rho) = 0, \quad (12)$$

where we have assumed that the energy is much smaller than the potential. The equation has two linearly independent solutions,

$$\sqrt{\rho} \rho^{\pm is} = \sqrt{\rho} e^{\pm is \ln \rho}, \quad (13)$$

or, equivalently,

$$\sqrt{\rho} \sin(s \ln \rho), \quad \sqrt{\rho} \cos(s \ln \rho). \quad (14)$$

The three-body system with zero-range potentials must be regularized [11] at some short-range scale r . The regularized wave-function at $\rho \ll |a_1|$ thus takes the form

$$\rho^{-\frac{1}{2}} f(\rho) = \sin\left(s \ln \frac{\rho}{r}\right). \quad (15)$$

2.3 Qualitative solution to hyper-radial equation

A qualitative solution to the hyper-radial equation can be obtained analytically by assuming that the two asymptotic solutions — being exact correspondingly at $\rho \gg |a_1|$ and $\rho \ll |a_1|$ — are qualitatively correct also in the region $\rho \sim |a_1|$. The phase-shift δ can then be obtained by matching the two asymptotic solutions at ρ_0 where attraction turns into repulsion.

At $\rho = \rho_0$ the short-distance function (15) arrives with the logarithmic derivative

$$\left. \frac{\frac{\partial}{\partial \rho}(\rho^{-\frac{1}{2}} f)}{(\rho^{-\frac{1}{2}} f)} \right|_{\rho=\rho_0} = \frac{s}{\rho_0} \cot\left(s \ln \frac{\rho_0}{r}\right) = \frac{s}{\beta|a_1|} \cot\left(s \ln \frac{\beta|a_1|}{r}\right), \quad (16)$$

where the factor $\beta = \rho_0/|a_1|$ is given as

$$\beta = \begin{cases} 0.84 & , \text{ for one-species system ;} \\ 0.29 \left(\frac{m_1}{m_3} \right)^{0.69} & , \text{ for two-species systems .} \end{cases} \quad (17)$$

This boundary condition causes the known log-periodic behavior of certain observables — as function of scattering length — in three-body systems with large scattering lengths.

Matching the short-range and the long-range solutions at $\rho = \rho_0$ gives the equation to determine the phase-shift δ ,

$$\kappa \frac{J'_2(\kappa\rho) - \tan(\delta)Y'_2(\kappa\rho)}{J_2(\kappa\rho) - \tan(\delta)Y_2(\kappa\rho)} = \frac{s}{\beta|a_1|} \cot \left(s \ln \frac{\beta|a_1|}{r} \right), \quad (18)$$

where the prime denotes the derivative of the Bessel function with respect to its argument.

In the following we shall only be interested in the recombination rate at zero temperature, that is, at vanishing energies, $\kappa \rightarrow 0$. In this regime the Bessel functions can be expanded as

$$J_2(z \rightarrow 0) = \frac{1}{8}z^2, \quad Y_2(z \rightarrow 0) = -\frac{4}{\pi}z^{-2}, \quad (19)$$

and then the phase-shift in the low-energy limit is given as

$$\tan(\delta) \approx \delta \approx (\kappa\beta|a_1|)^4 \frac{\pi}{32} \frac{1 - \frac{1}{2}s \cot \left(s \ln \frac{\beta|a_1|}{r} \right)}{1 + \frac{1}{2}s \cot \left(s \ln \frac{\beta|a_1|}{r} \right)}. \quad (20)$$

3 Recombination rate

3.1 Reaction rate in terms of hyper-spherical phase-shift

The long-distance hyper-radial solution (9) in the limit $\rho \rightarrow \infty$ becomes

$$f(\rho \rightarrow \infty) \rightarrow \sqrt{\frac{2}{\pi\kappa\rho}} \frac{e^{-i\kappa\rho+i\phi} + S e^{+i\kappa\rho-i\phi}}{2}, \quad (21)$$

where ϕ is a real number and $S \doteq e^{2i\delta}$.

If δ is a real number then $|S|^2 = 1$ and the hyper-radial flux density,

$$j = -i \frac{\hbar}{2m} \left(f^* \frac{\partial f}{\partial \rho} - \frac{\partial f^*}{\partial \rho} f \right), \quad (22)$$

vanishes – there is no loss of probability if the phase-shift δ is real.

However, a complex phase shift, $\delta = \Re\delta + i\Im\delta$, leads to a missing flux density,

$$\Delta j = \frac{\hbar\kappa}{m} \frac{1 - |S|^2}{2\pi\kappa\rho}, \quad (23)$$

where

$$1 - |S|^2 = 1 - e^{-4\Im\delta} \approx 4\Im\delta. \quad (24)$$

The total missing flux is obtained by integrating over the hyper-sphere. The integration element can be obtained from the relation

$$\frac{(dV)^2}{d\rho} = \left(\frac{1}{\mu_i \mu_{jk}} \right)^{3/2} \frac{d^3 x_i d^3 y_i}{d\rho} = m^3 \left(\frac{\sum m_i}{\prod m_i} \right)^{3/2} \rho^5 d\Omega_\rho, \quad (25)$$

where dV is the three-dimensional volume element and $\int d\Omega_\rho = \pi^3$. Besides this mass factors we also need to collect the (square of the) factor in front of $J_2(\kappa\rho)$ from the hyper-spherical expansion of the three-body plane-wave, normalized to unity within three-dimensional volume V ,

$$\frac{1}{V} e^{i\mathbf{k}_x \cdot \mathbf{x} + i\mathbf{k}_y \cdot \mathbf{y}} = \frac{1}{V} \frac{(2\pi)^3}{(\kappa\rho)^2} \left(\frac{1}{\pi^3} \right) J_2(\kappa\rho) + \dots, \quad (26)$$

where $\mathbf{k}_x^2 + \mathbf{k}_y^2 = \kappa^2$ and $\mathbf{x}^2 + \mathbf{y}^2 = \rho^2$.

Collecting all factors gives the following expression for the probability loss ΔJ per unit time — or recombination rate — within volume V ,

$$\Delta J = \frac{1}{V^2} m^3 \left(\frac{\sum m_i}{\prod m_i} \right)^{3/2} 2^5 \pi^2 \frac{\hbar}{m} \frac{1 - |S|^2}{\kappa^4}. \quad (27)$$

The factor $V^2 \Delta J$, often referred to as recombination constant K , can be written in terms of the three-body energy $E = \hbar^2 \kappa^2 / (2m)$ as

$$V^2 \Delta J = m^3 \left(\frac{\sum m_i}{\prod m_i} \right)^{3/2} 8 \pi^2 \frac{\hbar^5}{m^3} \frac{1 - |S|^2}{E^2}, \quad (28)$$

directly determines the recombination coefficients in the density balance equations for cold gases.

3.2 Recombination rate in zero-range model

In the zero-range model, where deep dimers are absent, the description of recombination into deep dimers, unlike recombination into shallow dimer, requires one extra parameter to make the phase-shift δ complex. This must be a short-range parameter as, indeed, to recombine into deep dimers all three atoms need to be at short-distances from each other — inside the range of their short-range potentials. This is also the region where the regularization of the zero-range three-body model takes place. Therefore the recombination range should be close to the regularization range r . The loss of probability — absorption — at short distances can be described by adding an imaginary part to the boundary condition at the regularization range. The easiest way to achieve this is to make the regularization parameter r complex,

$$r \rightarrow r e^{-i\epsilon}. \quad (29)$$

The absorption parameter ϵ determines the extent of the absorption.

Inserting the complex regularization radius (29) into the expression for the phase-shift (20), then the phase-shift into expression (24) for $1 - |S|^2$, and the latter, finally, into the recombination rate (28) gives the following expression for the recombination rate into deep dimers in our complex-boundary-condition zero-range model,

$$V^2 \Delta J = m^3 \left(\frac{\sum m_i}{\prod m_i} \right)^{3/2} 2^5 \pi^2 \frac{\hbar}{m} \beta^4 |a_1|^4 \frac{\pi}{8} \Im \frac{1 - \frac{1}{2} s \cot \left(s \ln \frac{\beta |a_1|}{r} + i s \epsilon \right)}{1 + \frac{1}{2} s \cot \left(s \ln \frac{\beta |a_1|}{r} + i s \epsilon \right)}. \quad (30)$$

The expression has two phenomenological parameters — the regularization range r and the absorption intensity at short distances ϵ . These parameters cannot be determined within the zero-range model and should be obtained by fitting the expression to experimental data.

For one-species system the shapes of recombination rates as function of scattering length for different absorption parameters are shown on Fig. 4. For small absorption parameter the log-periodic peaks caused by the term $s \ln(|a_1|/r)$ factor are well formed. Increasing the absorption smears the peaks out until they eventually disappear completely.

Two-species systems show similar smearing out of the log-periodic peaks with increasing the absorption parameter. However, the shape of the rate is also influenced by the heavy-to-light mass ratio, as illustrated on Fig. 5: increasing the mass ratio decreases the distance between the peaks and also increases the overall scale of the rate.

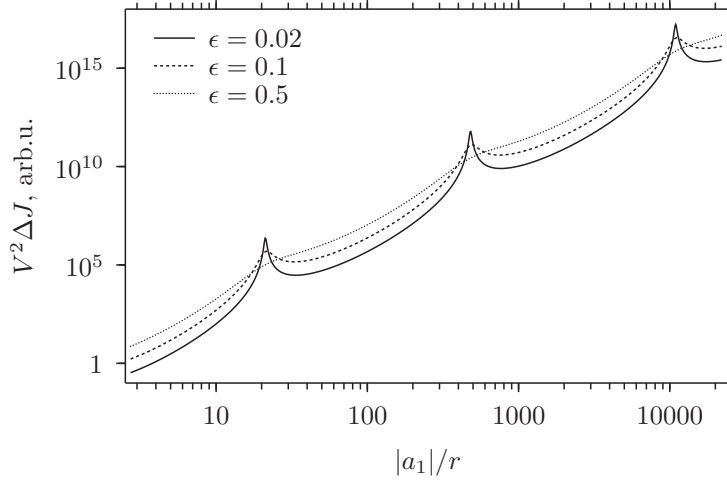


Fig. 4 The recombination rate $V^2 \Delta J$ (30) into deep dimers at zero temperature as function of scattering length a_1 for different values of the absorption parameter ϵ for one-species system.

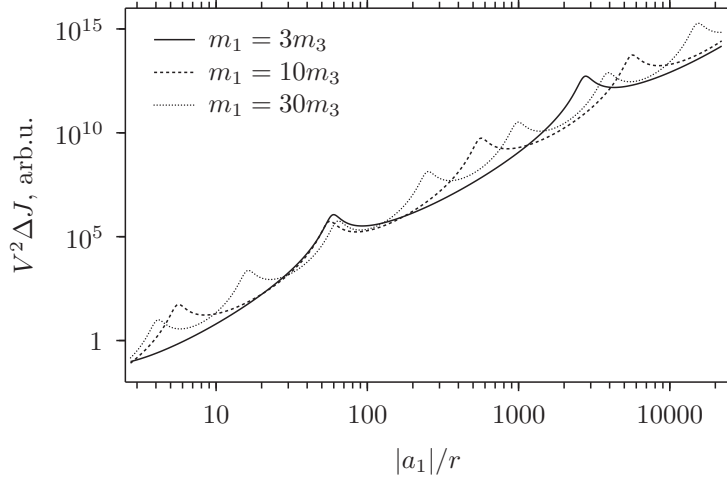


Fig. 5 The recombination rate $V^2 \Delta J$ (30) into deep dimers at zero temperature as function of scattering length a_1 for $\epsilon = 0.1$ and different values of the heavy-to-light mass ratio parameter m_1/m_3 for two-species systems.

4 Conclusion

We have investigated universal properties of the three-body recombination reaction rates into deep dimers within the zero-range hyper-spherical adiabatic approximation. Although a zero-range model cannot describe the deep dimers, it can still account for this reaction by introducing one extra parameter, which describes short-range absorption — or loss of probability — in the hyper-radial equation.

We have used a qualitative analytic solution of the hyper-radial equation comprised of the short- and long-range asymptotic solutions matched at the middle. This resulted in an analytic expression for the recombination rate as function of scattering length and the absorption parameter. We have given the expressions for both one- and two-species cold gases, the latter with one light and two identical heavy particles.

For weak absorption the recombination rate as function of scattering length shows characteristic log-periodic peaks. Increasing the absorption broadens the peaks until they are eventually smeared out.

For a meaningful comparison with experimental data the effects from the scattering length between the heavy particles need to be included [7]. The third scattering length modifies both the s and

β parameters in the expression for the recombination rate in a non-trivial way through significant modification of the eigenvalue equation. This should be a subject of a separate investigation.

A Hyper-spherical coordinates

Given the particle coordinates \mathbf{r}_i and masses m_i , where $i \in \{1, 2, 3\}$, the Jacobi coordinates are defined as

$$\mathbf{x}_i = \sqrt{\mu_i}(\mathbf{r}_j - \mathbf{r}_k), \quad \mathbf{y}_i = \sqrt{\mu_{jk}} \left(\mathbf{r}_i - \frac{m_j \mathbf{r}_j + m_k \mathbf{r}_k}{m_j + m_k} \right) \quad (31)$$

where

$$\mu_i = \frac{1}{m} \frac{m_j m_k}{m_j + m_k}, \quad \mu_{jk} = \frac{1}{m} \frac{m_i(m_j + m_k)}{m_i + m_j + m_k}. \quad (32)$$

where m is an arbitrary mass-scale.

The hyper-angular coordinates are the hyper-radius, ρ , defined as

$$\rho^2 \doteq \mathbf{x}_i^2 + \mathbf{y}_i^2 = \frac{\sum_{i < k} m_i m_k (\mathbf{r}_i - \mathbf{r}_k)^2}{m(m_1 + m_2 + m_3)}, \quad (33)$$

and five hyper-angles, Ω_ρ ,

$$\Omega_\rho \doteq \left\{ \alpha_i \doteq \arctan \left(\frac{x_i}{y_i} \right), \frac{\mathbf{x}_i}{x_i}, \frac{\mathbf{x}_i}{y_i} \right\}. \quad (34)$$

For identical particles the index can be omitted.

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